WORKSHOP ON

"Total Least Squares: Concepts, Algorithms, Applications".

Leuven-Heverlee, Belgium,
August 12-15, 1991.

FINAL PROGRAM :

- time schedule
- abstracts
- list of participants

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HOSTED BY :

ESAT Laboratory, Department of Electrical Engineering,
Katholieke Universiteit Leuven, Kardinaal Mercierlaan 94, 3001 Heverlee, Belgium.

ORGANIZING COMMITTEE :

- *Sabine Van Huffel*
  Department of Electrical Engineering, Katholieke Universiteit Leuven, Heverlee, Belgium.
- *Bart De Moor*
  Department of Electrical Engineering, Katholieke Universiteit Leuven, Heverlee, Belgium.
- *Gene Golub*
  Department of Computer Sciences, Stanford University, Stanford, U.S.A.

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- Leuven Measurement & Systems (LMS) International.

WORKSHOP ON

"Total Least Squares: Concepts, Algorithms, Applications".

August 12-15, 1991.

PROGRAM

and

TIME SCHEDULE

All sessions are held in :

auditorium Arenberg, Arenberg castle,
Kardinaal Mercierlaan 94, 3001 Heverlee, Belgium.

Monday, August 12

12.30-13.45	*Lunch in salons Arenberg, Arenberg castle*	Page
13.45-14.00	*Opening of the Workshop*	
Session 1 :	**Basic concepts of the TLS problem**	
14.00-14.30	*Gene H. Golub* Basic principles of the TLS problem	26
14.30-15.30	*Sabine Van Huffel* The TLS problem: current state of research and applications	42
15.30-16.00	*Break*	
Session 2 :	**Structured and constrained TLS problems**	
16.00-16.30	*James Demmel* TLS with structured perturbations	20
16.30-17.00	*Bart De Moor* Structured TLS problems	21
17.00-17.30	*Theagenis J. Abatzoglou* Constrained TLS and superresolution signal processing	11
17.30-18.00	*James A. Cadzow* Constrained TLS problem	17
19.00	*Dinner in restaurant "De Oude Kantien"*	

Tuesday, August 13

15.30-16.00 *Break*

Session 6 : Errors-in-variables and statistical properties, part 2

16.00-16.30 *Chi-Lun Cheng* 18
TLS and errors-in-variables regression

16.30-17.00 *Larry P. Ammann* 13
Algorithms for robust M-estimation of covariance eigen-structure

17.30-19.30 *Guided visit through Leuven: beguinage, city hall, university*

20.00 *Dinner in restaurant "De Oude Kantien"*

Wednesday, August 14

Session 7 : Errors-in-variables and system identification

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09.00-09.30	*Torsten Söderström* Some aspects on treating measurement errors in system identification	37
09.30-10.00	*Roberto P. Guidorzi* Errors-in-variables identification and model uniqueness	27
10.00-10.30	*Adina Stoian* Comparative performance study of least squares and TLS Yule-Walker estimates of autoregressive parameters	39
10.30-11.00	*Break*	

Session 8 : TLS applications in signal processing

11.00-11.30	*Donald W. Tufts and Abhijit A. Shah* Signal enhancement motivated by TLS and linear prediction	40
11.30-12.00	*Richard Roy* Real world applications of TLS: Direction-finding and system identification	35
12.00-12.30	*Michael P. Clark and Louis L. Scharf* Maximum likelihood parameter estimation for array processing	19
12.30-14.00	*Lunch in salons Arenberg, Arenberg castle*	

Session 9 : Nonlinear TLS problems

14.00-14.30	*Yasuo Amemiya* Parameter estimation in nonlinear errors-in-variables problems	12
14.30-15.00	*Paul T. Boggs* Orthogonal distance regression	15
15.00-15.30	*Janet E. Rogers* ODRPACK: software for orthogonal distance regression	34

15.30-16.00 *Break*

Session 10 : Other TLS applications

18.00-19.00 *Demonstrations*

19.30 *Banquet*

Thursday, August 15

WORKSHOP ON

"Total Least Squares: Concepts, Algorithms, Applications".

August 12-15. 1991.

ABSTRACTS

Constrained Total Least Squares Problem and Superresolution Signal Processing.

Theagenis J. Abatzoglou

Lockheed Missiles & Space, Inc.,
Research & Development O/91-50, B251,
3251 Hanover Street, Palo Alto, CA 94304-1191, U.S.A.

Constrained Total Least Squares (CTLS) is a generalized version of Total Least Squares where the noise perturbations to the coefficients of a linear system of equations are allowed to satisfy linear relations. Theoretical properties of the CTLS solution are presented which include its equivalence to a Maximum Likelihood estimator, reduction of the solution to an unconstrained lower dimensionality problem, perturbation analysis and numerical algorithms.

Applications of CTLS to signal processing are realized by imposing a linear model to data samples. Linear prediction is a good model for harmonic signals; applications include: frequency estimation (one- or two-dimensional), direction finding, extraction of resonances of objects, etc.

Parameter Estimation in Nonlinear Errors-in-Variables Problems.

Yasuo Amemiya

Department of Statistics, Iowa State University, 102G Snedecor Hall, Ames, Iowa 50010, U.S.A.

The functional errors-in-variables model assumes that observations are the sums of underlying true values and measurement errors, and that the true values are fixed constants satisfying some relationship. The case where the relationship is specified by a nonlinear parametric function is considered. The maximum likelihood estimator of the parameter under the assumption of normal measurement errors is a nonlinear total least squares estimator. It is shown that such an estimator has a nonnegligible bias due to the nonlinearity and measurement errors. An estimator that does not have such a bias is suggested. Theoretical and numerical results supporting the superiority of the bias-adjusted estimator relative to the maximum likelihood estimator are presented.

Algorithms for Robust M-Estimation of Covariance Eigen-structure.

Larry P. Ammann

Programs in Mathematical Sciences,
University of Texas at Dallas,
Richardson, TX 75080, U.S.A.

Robust location and covariance estimators are developed via general M-estimation for covariance matrix eigenvectors and eigenvalues, which results in a generalization of projection pursuit. The solution to this M-estimation problem is obtained by transforming it into a series of robust regression problems. The motivation for this transformation is the interpretation of the singular value decomposition as an iteration of two steps — a least squares regression fit of the data matrix followed by a rotation to the regression hyperplanes. An algorithm to obtain this solution is presented, along with results of a Monte Carlo study and examples of its application.

This algorithm is derived by efficiently replacing least squares regression with robust regression, which then produces a broad class of new robust methods for multivariate data. Some results in numerical linear algebra are presented which describe the relationships among least squares regression, the QR decomposition, and the singular value decomposition. These results are utilized in the algorithm to solve the M-estimation problem so that it can be built upon standard, commonly available, numerical linear algebra routines. In addition, it is shown how the output of this algorithm can be used to search numerically for multivariate outliers. This is especially useful in exploratory data analysis with high-dimensional data where graphical techniques are difficult to implement. Since the algorithm computes robust estimates of the eigenvectors and eigenvalues of the covariance matrix, it can be used as a basis for other multivariate methods such as signal subspace estimation and direction of arrival problems, errors-in-variables regression, discriminant analysis, and principal components. The examples of its application given here include some data sets which have been examined by other methods for comparison purposes, and an application to a large data set taken from the Landsat satellite.

Infinite Dimensional Total Least Squares Problems.

K. S. Arun

Coordinated Science Laboratory,
University of Illinois,
1101 West Springfield Avenue,
Urbana-Champaign, IL 61801, U.S.A.

In this lecture, we will formulate and solve infinite dimensional versions of the generic and non-generic total least squares problems, and apply it to problems such as deconvolution, linear-min-variance estimation, system identification, and Kalman and Wiener filtering.

Orthogonal Distance Regression.

Paul T. Boggs

National Institute of Standards and Technology (NIST),
Applied and Computational Mathematics Division,
Gaithersburg, MD 20899, U.S.A.

We describe the Orthogonal Distance Regression problem (ODR), i.e., the problem of fitting a function to a given set of data, $(x(i), y(i))$, $i = 1, \ldots, n$, where errors are assumed to exist in both the x-values as well as in the y-values. This is in contrast to ordinary least squares (OLS) where all of the errors are assumed to exist in the y-values. We first precisely define the (ODR) problem, and then briefly describe a stable and efficient algorithm for its solution; the algorithm and its implementation in the software library ODRPACK, as well as examples that have arisen at NIST, will be discussed in detail by J. Rogers. Here, we will concentrate on simulation studies that compare ODR to OLS in a controlled setting. In particular, we compare ODR with OLS under the assumption that the ratio of the errors in y to the errors in x is known. Several measures of performance are considered. We then relax this assumption and compare the performance of ODR when the ratio is not known precisely. Finally, we discuss the computation and use of the asymptotic covariance matrix.

Collinearity and the One-Dimensional Total Least Squares Problem.

James R. Bunch and Ricardo D. Fierro
Department of Mathematics,
University of California a' San Diego,
La Jolla, CA 92093-011z, U.S.A.

The numerical effects of collinearity in the columns of A on the TLS estimator will be considered. The TLS problem can become ill-conditioned and a regularization technique is employed to stabilize the solution by increasing the dimension of the solution space. A condition estimator for the new, but related, problem is proposed; it coincides with the condition number in the generic case. An approximation theorem will be presented which more formally specifies the near-intimate relationship between SVD components of A and $[A, b]$ when $v_{n+1,j}$, the last component of the jth right singular vector of $[A, b]$, is "small". For example, this arises when the jth singular value of $[A, b]$ is nonpredictive.

The smallest singular values of $[A, b]$ inherited from A may identify collinearities that are all predictive, or all nonpredictive, or a combination of both. We will present a theorem which implies that one should deduce a minimum norm solution in a space that includes the singular vectors associated with the collinearities inherited from A, regardless of their predictive value. Intuitively, when the clustered singular values are included, the solution space is more "stable".

We will compare the TLS solution to the Truncated LS solution of $Bx = b$, where B is the nearest rank r approximation to A. We will discuss how the regularized TLS solution is also the unique minimum norm solution to a particular LS problem that has a higher condition number than the Truncated LS problem of the same dimension. Although the matrix can differ in its singular values and singular vectors from those of B, the singular triplets associated with the largest singular values are usually close to the corresponding ones of B.

Constrained Total Least Squares Problem.

James A. Cadzow
Department of Electrical Engineering,
Vanderbilt University,
P.O.Box 6080, STA. B, Nashville, Tennessee 37235, U.S.A.

In the standard total least squares problem, one is given a system of inconsistent linear equations

$$e = Ax - b$$

in which the matrix A and vector b are subject to error. It is now desired to perturb the system matrix A to $A + E$ and the vector b to $b + r$ so that

1. $[A + E]x = b + r$ is consistent
2. of all such modifications, the perturbations used have minimum Euclidean norm.

In many applications, the underlying noise free matrix $[A; b]$ will possess theoretical properties such as having a specific structure (e.g., Toeplitz) and a given rank. In order to retain these properties, the perturbations E and r need be appropriately constrained. In this presentation, an algorithm is presented for achieving the minimum Euclidean perturbation so that the perturbed system of equations possesses the required properties.

Total Least Squares and Errors-in-Variables Regression.

Chi-Lun Cheng

Institute of Statistical Science,
Academia Sinica, Taipei, Taiwan, R.O.C.

This talk surveys the problem of total least squares from a theoretically statistical viewpoint. It includes the errors-in-variables model and principal component analysis which are numerically equivalent to total least squares under certain assumptions. We also discuss the robust version of the statistical models corresponding to total least squares.

Maximum Likelihood Parameter Estimation for Array Processing.

Michael P. Clark and Louis L. Scharf
Department of Electrical and Computer Engineering,
University of Colorado,
Campus Box 425, Boulder, CO 80309-0425, U.S.A.

We use the data collected by a multisensor array to identify the Directions Of Arrival (DOA), frequency and amplitude of individual point sources in the far-field. Many methods for solving this problem have been developed. However, most of these methods work only for sources with the same center frequency. Those which do allow arbitrary frequencies can predict both the frequencies and the DOAs. However, these methods have difficulty associating (pairing) the frequencies and DOAs. We propose an algorithm, based on the principle of maximum likelihood, which solves the "pairing" problem for arrays with linear geometries. The method works by identifying a matrix which characterizes the orthogonal subspace. This matrix has two parts. The first of these is based on a temporal, whitening polynomial. The second uses an interpolating polynomial which predicts spatial modes from temporal modes. The method works by solving for the parameters which chararcterize the orthogonal subspace, making it a subspace method. The orthogonal subspace is identified by any of several methods, including least squares and total least squares. Once the parameters of the orthogonal subspace have been estimated, the temporal polynomial is rooted to obtain the temporal modes. These modes are then plugged into an interpolating polynomial to generate the corresponding spatial modes. Simple geometrical considerations then yield the DOA estimates.

Total Least Squares with Structured Perturbations.

James Demmel

University of California at Berkeley,
Computer Science Division,
Evans Hall 513, Berkeley, CA 94720, U.S.A.

The classical TLS solution of $AX = B$ involves using the SVD to find a nearest rank deficient matrix to $[A, B]$. This treats errors in all entries of A and B equally. One often wants to impose more structure on perturbations in A and B. Previous work has imposed row and column scalings or block structures on the perturbations. We discuss imposing an independent error scaling on each entry of A and B; i.e. the error norm is not given by a ball but by an arbitrary rectangular parallelepiped. We discuss recent results of Rohn and Poljak who give a solution for a certain special case, and show that even in this special case the problem is NP-complete. Recent work on approximating this NP-complete solution as well as open problems are discussed.

Structured Total Least Squares Problems.

Bart De Moor[1]
Katholieke Universiteit Leuven,
ESAT Laboratory, Department of Electrical Engineering,
Kardinaal Mercierlaan 94, B-3001 Heverlee, Belgium

Given a real matrix $A \in \Re^{p \times q}$ with $p \geq q$ and $rank(A) = q$. Let A be decomposed as $A = F + M$ where F contains the elements that cannot be modified and M contains the elements to be modified. The zero patterns in F and M are complementary: $f_{ij}m_{ij} = 0$. The *structured total least squares problem* is the problem of finding a rank deficient matrix $B = F + N$ so that $\|M - N\|_F^2$ is minimized and the zero pattern of N is complementary to that of F: $n_{ij}f_{ij} = 0$.

When $F = 0$, the problem is known as the *total least squares problem* [4] and is solved using the singular value decomposition [3]. Solutions for some specially structured matrices A have been obtained, such as a matrix A with 'exact' columns (i.e. where F is of the form $F = [\ F_1 \ \ 0\ ]$) [5] or when only the lower right hand corner block of a four block partitioned matrix A can be modified [1] [2]. It remains unsolved however in full generality.
We provide some more insight by showing that the solution is equivalent with solving a special type of SVD completion problem.

We also derive a remarkable correspondence between the structured TLS problem where A is four block partitioned and three out of four blocks can be modified, and the solution to the following total least squares problem with three matrices: Given $A \in \Re^{k \times l}$, $B \in \Re^{m \times n}$ and $C \in \Re^{k \times n}$. Find $X \in \Re^{l \times m}$ so that the object function $\|A-P\|_F^2+\|B-Q\|_F^2+\|C-R\|_F^2$ is minimized subject to $PXQ = R$. A solution for the scalar case where A is a column vector and B a row vector has been obtained recently and will probably be generalized by the time of the workshop.

References

[1] J.W. Demmel, *The smallest perturbation of a submatrix which lowers the rank and constrained total least squares problems.* SIAM J. Numer. Anal. 24 (1987), pp. 199-206.

[2] B. De Moor and G.H. Golub, *The restricted singular value decomposition: properties and applications.* SIAM J. Matrix Anal. Appl. 12, no.3, July 1991.

[1]Research Associate of the Belgian N.F.W.O. (National Fund for Scientific Research)

[3] C. Eckart and G. Young, *The approximation of one matrix by another of lower rank.* Psychometrika 1 (1936), pp.211-218.

[4] G.H. Golub and C.F. Van Loan, *An analysis of the total least squares problem.* SIAM J. Numer. Anal. 17 (1980), pp. 883-893.

[5] G.H. Golub, A. Hoffman and G.W. Stewart, *A generalization of the Eckart-Young-Mirsky matrix approximation theorem.* Lin. Alg. Appl. 88/89 (1987), pp. 317-327.

Total Least Squares Methods of Analyzing Mineral Assemblages and Reactions in Metamorphic Rocks.

George W. Fisher

Department of Earth and Planetary Sciences,
The Johns Hopkins University,
Baltimore, Maryland 21218, U.S.A.

Interpretation of mineral assemblages in metamorphic rocks depends upon determining

1. whether or not individual assemblages could represent equilibrium states;
2. whether or not pairs of assemblages could have equilibrated under the same pressure, temperature conditions; and
3. the nature of the reactions relating assemblages equilibrated under different conditions.

Traditional methods of analysis rely on graphical projection methods which are simple to use, but can not deal effectively with assemblages involving variation in more than three components. In multicomponent assemblages, these questions are best approached by investigating the rank, composition space (range) and reaction space (null space) of matrices in which the phases of an assemblage are represented by columns and the components by rows.

Total Least Squares (TLS) methods based on the singular value decomposition provide a simple and elegant way of finding a model matrix of specified rank which approximates the observed matrix within analytical uncertainty. Examination of the elements of the null space (or reaction space) associated with that matrix provide unambiguous criteria for identifying possible equilibrium assemblages and for determining whether or not two assemblages can have equilibrated under the same external conditions: an empty null space reflects a possible equilibrium assemblage; a null space containing reactions in which the minerals of two assemblages have opposite signs indicates that the two assemblages intersect in composition space and therefore can not have equilibrated under the same conditions; a null space lacking any such reactions indicates that the two assemblages do not intersect, and so may have equilibrated under the same conditions.

I have developed a set of easy-to-use computer programs which perform these operations. Trial runs using analyzed mineral compositions from three outcrops spanning the lower sillimanite zone of northwestern Maine, described by C.T. Foster (1977, Am. Mineralogist) illustrate the power of the method. All assemblages contain the seven phases sillimanite, staurolite, biotite, garnet, muscovite, quartz, plagioclase and ilmenite. All assemblages examined have a rank of seven, requiring seven components, and probably represent divariant equilibrium. Assemblages from individual outcrops show no significant intersections, while those from outcrops differing in temperature by as little as 6° C show systematic intersections reflecting divariant reactions.

Properties of Estimators for the Errors-in-variables Model.

Wayne A. Fuller

Department of Statistics, Iowa State University, Snedecor Hall, Ames, Iowa 50010, U.S.A.

The method of total least squares can be used to produce estimates of the parameters of a statistical model. For the linear model, the properties of the estimators can be derived under relatively weak assumptions. We give conditions sufficient for the estimators to be statistically consistent. Also, an estimator of the covariance matrix of the limiting distribution of the estimated parameter vector is presented. The estimation procedures have been implemented in a personal computer program.

Basic Principles of the Total Least Squares Problem.

Gene H. Golub

Department of Computer Sciences,
Stanford University,
Stanford, CA 94305, U.S.A.

We review some of the basic ideas and principles involved in the development of Total Least Squares.

Errors-in-variables Identification and Model Uniqueness.

Roberto P. Guidorzi

Diparttimento di Elettronica, Informatica e Sistemistica,
Università di Bologna,
Viale del Risorgimento 2, 40136 Bologna, Italy

The problem of deriving possible linear relations from data affected by additive noise has received remarkable attention in recent years particularly regarding the assumptions ("prejudices") behind the procedures leading to unique models. Unlike the many approaches leading to unique solutions (Least Squares, Maximum Likelihood, etc.) the Frisch scheme, belonging to the family of Errors-in-Variables (EV) schemes, leads to a whole family of models compatible with a set of noisy data and is considered as only mildly affected by prejudices.

This talk discusses the loci of all possible solutions, in the noise space, under the assumptions of the Frisch scheme and shows how it can be possible, when different sets of noisy data are available, to obtain the unique model behind the data and also to derive the actual amount of noise on the data when the noiseless data are linked by a single linear relation. The more general EV case of non-independent additive noises is then considered and it is shown how, under the same assumptions, it is still possible to obtain the unique set of parameters linking the noiseless data and the whole family of compatible noise covariance matrices which is defined, in this case, by the infinite elements of a linear variety.

Finally, the previous considerations, which regard algebraic systems, are extended to dynamic systems; in this case, the dimensions of the noise and parameter spaces are no longer equal and also the order of the model must be estimated. Also in this case, procedures can be developed for a consistent estimation of the model order and the parameters and for the estimation of the noise covariance matrix.

A Model for Signature Verification.

Trevor Hastie, Eyal Kishon, Malcolm Clark and Jason Fan
AT&T Bell Laboratories,
600 Mountain Avenue, Murray Hill, NJ 07974, U.S.A.

We propose a statistical model for dynamic signature verification by computer. Our model recognizes that repeated signatures by the "owner" are similar but not identical. Our model consists of a *template* signature for each individual, and several factors which allow for variations in each rendition of this template. These variations include the *speed* of writing, as well as slowly varying affine transformations such as size, rotation and shear. The estimated template represents the "mean" of a sample of signatures from an individual, and the variations in the factors can be used to establish several measures of "variance". These quantitative measures are essential for reliable signature verification.

Estimating the template consists of two essential steps:

- Aligning or "time-warping" the set of realized signatures for an individual, and segmenting all the signatures into "letters",
- given the alignment and segmentation, estimating the average shape of the signatures using piece-wise affine-invariant TLS.

A new signature is verified by comparing it with the template signature. It will be judged fraudulant if its shape is wrong, or if the speed signal with which it was rendered does not match the model. In this talk I describe the model and its estimation, illustrating the procedures with several examples.

Principal Curves.

Trevor Hastie

AT&T Bell Laboratories,
600 Mountain Avenue, Murray Hill, NJ 07974, U.S.A.

Tom Duchamp

Department of Mathematics,
University of Washington,
Seattle, WA 98195, U.S.A.

Werner Stuetzle

Department of Statistics,
University of Washington,
Seattle, WA 98195, U.S.A.

Principal curves are smooth one-dimensional curves that pass through the middle of a p-dimensional dataset, providing a nonlinear summary of the data. They are nonparametric, and their shape is suggested by the data. In this talk I will define principal curves, discuss algorithms for their construction, present theoretical results, and illustrate their application.

The Use of Total Least Squares in an Oceanographic Problem.

Jae Hak Lee

Department of geology and geophysics,
Yale University,
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An appealing property of the total least squares (TLS) solution is its invariance to some cases of transformations of unknowns. That is, for an overdetermined set of linear equations **Ax**=**b** where **A** is the coefficient matrix, **b** is the data vector and **x** is the vector of unknowns, the TLS solution is not affected by the rotation of the space of **A** and **b** or a reciprocal transformation of unknowns. The latter case is used to treat a special problem which has no inhomogeneous term (i.e., **b**=**0**) but with *a priori* information. It is shown that, unlike the ordinary least squares method, the TLS method yields a unique set of solutions. As an application of this property to real situations, the TLS method is applied to an oceanographic inverse problem which is to determine velocities and diffusion coefficients from known tracer (temperature and salinity here) distributions based on the steady-state advective-diffusive equation and mass continuity. The derived diffusivities lead to conclusions that are consistent with the known physics. This indicates that the application of TLS is quite successful.

We review the invariance of the TLS solution by using a geometric interpretation of the line fitting problem and report the results of this successful application of the TLS method.

Total Least Squares and Acceptable/ Generalized Solution to a Problem. Theoretical Results for General Norms.

Jean-François Maitre

Ecole centrale de Lyon,
Departement de Mathématiques,
B.P. 163, 69131 Ecully cedex, France

We consider a problem in the form

$$x \in E,\ P(x) = 0, \tag{1}$$

where P is a mapping from a set E to a linear space F and a normed linear subspace $\mathcal{A}$ of F^E. For each $x \in E$, we define

$$e(x) = \inf\{\|\delta P\|; \delta P \in \mathcal{A}, (P + \delta P)(x) = 0\}. \tag{2}$$

We say that x is an ε-solution to (1) if $\delta P \in \mathcal{A}$ exists with

$$(P + \delta P)(x) = 0,\ \ \delta P < \varepsilon, \tag{3}$$

which is equivalent to $e(x) < \varepsilon$.

We say that x_0 is a generalized solution to (1) if

$$e(x_0) = \min\{e(x); x \in E\}. \tag{4}$$

The quantity $e(x)$, given by(2), is equal to $\|P(x)\|_x$, where the semi-norm $\|.\|_x$ is defined by:

$$\|y\|_x = \inf\{\|M\|; M \in \mathcal{A}, M(x) = y\}. \tag{5}$$

We give conditions of existence and properties of $\|.\|_x$. When E and F are normed linear spaces, $\mathcal{A}$ consists of linear mappings and $\|.\|_x$ is a norm for $x \neq 0$, we have the equivalence :

$$\forall x \in E \setminus \{0\}, y \in F, \|y\|_x = \|y\|/\|x\| \ \Leftrightarrow\ \forall x \in E, f \in F', \|f\|_x^* = \|x\|\|f\| \tag{6}$$

and $\mathcal{L}(E, F)$ is the greatest $\mathcal{A}$ for which the relations in (6) are right.

In the case of a linear problem

$$Ax - b = 0, \tag{7}$$

that is $P(x) = Ax - b$, and special choices of the norm of $\mathcal{A}$ satisfying (6), we have

$$e(x) = \|b - Ax\| / \|(x, 1)\| \tag{8}$$

which corresponds for the euclidean norm to the Total least Squares problem. When $\mathcal{A}$ is limited to perturbations $(0, \delta b)$ we have $e(x) = \|b - Ax\|$ (Least Squares), and when $\mathcal{A}$ is limited to perturbations $(\delta A, 0)$ we have $e(x) = \|b - Ax\| / \|x\|$.

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[2] J.F. MAITRE. Sur une classe de normes et l'analyse a posteriori d'un système linéaire. *Numer. Math.* 12 (1968), pp. 106-110.

[3] J.F. MAITRE. Problèmes voisins, solutions acceptables et solutions généralisées d'un problème. Séminaire, Université de Grenoble, et Colloque d'Analyse Numérique, Aussois, 1969, 26 pp.

Algorithms and Architectures for Recursive Total Least Squares Estimation.

Marc Moonen[2]

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ESAT Laboratory, Department of Electrical Engineering,
Kardinaal Mercierlaan 94, B-3001 Heverlee, Belgium

Total least squares parameter estimation is an alternative to least squares estimation, although much less used for instance in adaptive filtering. The absence of efficient recursive algorithms here has apparently been a motive for using Recursive Least Squares (RLS) even in those applications where typically one would better use the TLS technique. Our aim is therefore to derive a similar recursive total least squares (RTLS) algorithm, which is also amenable to parallel implementation. It turns out that a RTLS algorithm can be constructed, based on inverse iteration, which very much resembles the original RLS algorithm. Algorithmic and architectural considerations for RLS then straightforwardly carry over to the RTLS case.

[2]Senior Research Assistant of the Belgian N.F.W.O. (National Fund for Scientific Research)

ODRPACK: Software for Orthogonal Distance Regression.

Janet E. Rogers
National Institute of Standards and Technology (NIST),
Applied and Computational Mathematics Division,
325 Broadway, Boulder, Colorado 80303-3328, U.S.A.

We will examine the Orthogonal Distance Regression (ODR) technique for fitting data to a general nonlinear model when there are errors in all of the variables $(x(i), y(i))$, $i = 1, \ldots, n$. ODR solves this extended least squares problem by minimizing the sum of the squared orthogonal distances between each data point and the curve described by the model equation. The number of unknowns involved in the ODR problem is the number of model parameters plus the number of variables observed with measurement error, often a very large number. By exploiting the structure of the problem, however, we have developed a stable and efficient trust region Levenberg-Marquardt algorithm with a work per step bound equal to that required for the Levenberg-Marquardt method for ordinary least squares (OLS), where the number of unknowns is simply the number of model parameters.

We will describe our ODR algorithm, and also the use and features of the software library ODRPACK that is an implementation of it. ODRPACK can be used to solve explicit, implicit and multiresponse ODR problems. Our discussion will include several examples of such ODR problems that have arisen at NIST and that exemplify the performance of ODRPACK. P. Boggs will also provide examples of ODRPACK's use, showing the results of simulation studies that compare ODR to OLS in a controlled setting. The ODRPACK software will be available for demonstration and distribution.

Real World Applications of Total Least Squares: Direction-finding and System Identification.

Richard Roy

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Various aspects and experiences in the application of TLS concepts to the problems of direction-of-arrival (DOA) estimation and multivariable linear system identification will be discussed. A demonstration of several such applications to real data will be presented. These will include DOA estimation in a coherent source environment, and system identification of a large flexible space structure. A MATLAB Toolbox for sensor array signal processing (AP Toolbox) will be presented along with a similar set of routines for system identification. Some open/difficult problems remaining to be solved will be described and recent attempts at their solution outlined. These include exploitation of problem structure to reduce computational complexity, and the problem of detecting dimensionality of the appropriate subspaces in these problems.

Tensorial Calibration in Chemistry.

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One goal in analytical chemistry is to relate a series of readily acquired measurements to a physical or chemical property of a sample. Tensorial calibration is a context for characterizing the types of data produced by analytical instrumentation. Instruments measure (per sample) a response that is either a zeroth, first, second or third order tensor (scalar, vector, matrix or cube, respectively). The Total Least Squares (TLS) problem arises in first order calibration, when a vector of data is collected per sample, giving the model $c = Rb + \varepsilon$, where c is a vector containing the concentrations for all the samples, R is a matrix with the response for each sample in a row, and b is the regression vector.

A method called Parsimonious Regression (PR) will be presented that reduces the amount of measurement error in R incorporated into the model. This method starts with a principal component decomposition of R. Even the largest principal component factors (eigenvectors of RR^T and R^TR with large eigenvalues) will contain some measurement noise. This method eliminates one dimension (rank) at a time according to a cross validation criterion, which forces the parts of the eigenvectors corresponding to nonrelevant variance (measurement error) to be removed. Cross validation more closely models the predictive capability of a model than does the fit of the data used to make the model, and will not allow correlations of noise in R to c to be incorparated into the model. The one remaining dimension after the decomposition has been reduced to rank one and will point in the direction of the regression vector b. This method will be compared to principal component regression (PCR) and partial least squares (PLS). PCR and PLS minimize a least squares fit criterion with a single step projection, while in PR any criterion can be minimized.

Some Aspects on Treating Measurement Errors in System Identification.

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When applying system identification (modelling of dynamic systems) it is necessary to account for disturbances and measurement errors. Some different cases, like presence of input and output errors, are discussed, as well as their consequences for parameter fitting. It is demonstrated how a standard least squares fit does not give a consistent model when the output measurement noise is uncorrelated (white noise). A bias compensation can be used at a modest cost to give a consistent model. The method so constructed can also be interpreted as a classical eigenvector method or a total least squares fit. Its statistical properties are reviewed. The parameter estimates are consistent and asymptotically Gaussian distributed. Alternative identification methods, like instrumental variables and output error methods, are briefly discussed, and compared to the total least squares approach.

Updating Rank Revealing URV Decompositions.

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Let X be an $n \cdot p$ matrix and let x be a p-vector. In many applications it is required to determine the effective rank of

$$\hat{X} = \begin{pmatrix} X \\ x^{\mathrm{T}} \end{pmatrix}$$

and compute an approximate null space for $\hat{X}$. In general, the problem will have already been solved for X by means of a suitable decomposition. The problem is then to update this decomposition to obtain the corresponding decomposition of $\hat{X}$.

In many ways the decompositions of choice are the singular value decomposition of X or the spectral decomposition of $C = X^{\mathrm{T}}X$. However, both these decompositions are difficult to update. An alternative is the (pivoted) QR decomposition of X or the Cholesky decomposition of C, both of which can be updated. However, these decomposition do not provide an explicit basis for the approximate null space.

In this talk we describe a class of orthogonal decompositions, called URV decompositions, which in some sense lie between the singular value decomposition and the QR decomposition and share the advantages of both. They can be made rank revealing and they furnish an explicit basis for the approximate null space. Moreover, they can be updated sequentially in $O(p^2)$ time. On a linear array of p processors, they can be updated in $O(p)$ time.

Comparative Performance Study of Least Squares and Total Least Squares Yule-Walker Estimates of Autoregressive Parameters.

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This talk considers the estimation of the parameters of autoregressions from noisy measurements. A new method for solving this problem is presented, which uses a combination of two recent algorithms: a High-Order Yule-Walker (HOYW) algorithm for estimation of the autoregressive (AR) parameters of an autoregressive moving average (ARMA) model, introduced by P. Stoica, B. Friedlander and T. Söderström, and the Total Least Squares (TLS) algorithm studied by S. Van Huffel. Simulation results are presented in order to evaluate the proposed HOYW-TLS technique and the HOYW-LS technique with respect to their accuracy in parameter estimation of autoregressions. The performances of these two techniques are mainly influenced by the following factors: the pole-zero configuration of the ARMA processes, the sample length and the dimension of the HOYW system. It is concluded that the HOYW-TLS technique is especially useful for any sample length and any dimension of the HOYW system, when the zeros of the ARMA model are close to the unit circle. However, even if no information about the singularities of the ARMA process is available, the use of the TLS method is proved to be strongly recommended. for it is in practice never less accurate than the classical LS technique.

Signal Enhancement Motivated by Total Least Squares and Linear Prediction.

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Evaluation and improvement of a SVD-based data-adaptive signal estimation algorithm[1] are presented. In the first step of this algorithm a matrix with a Hankel-like structure is formed from the noise corrupted time-series data. It is assumed that the rank of the signal only data matrix is known or is obtainable from the Singular Value Decomposition (SVD) of the noise corrupted data matrix. What is important is that the signal only matrix can be well approximated by a matrix of lower rank. Using SVD such a low rank approximation of the signal only matrix is made. By summing across the diagonals of this "cleaned up" post-SVD low rank matrix, time series data with enhanced signal component is extracted.

The highly nonlinear nature of SVD makes performance evaluation of such SVD-based applications a difficult task, but methods of backward error analysis make the task easier. The best low rank approximation of a perturbed matrix is approximated by a first order perturbation expansion of the orthogonal subspace. This makes computation of statistical properties of the post-SVD data a tractable problem. Using the obtained statistical information, performance of the signal enhancement algorithm is evaluated.

It is also shown that this statistical information can be utilized to extract the enhanced signal from the post-SVD low rank matrix by an optimal linear combination of its elements. Computer simulation results for verifying theoretical predictions and for comparing the performance of the original and modified algorithms to the Cramér-Rao bound are presented.

References

[1] D.W. Tufts, R. Kumaresan, and I.P. Kirsteins, "Data Adaptive Signal Estimation by Singular-Value-Decomposition of a Data Matrix," *Proceedings of the IEEE*, vol. 70, no. 6, pp.687-685, June 1982.

Asymptotic Properties of a Class of Regression-type Estimators.

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An asymptotic analysis of the regression problem $Hp = 0$ where only a noisy observation G of H is available is presented. A class of estimators for p is given by the minimizer of $p^t G^t D_p^{-1} G p$ over p, where D_p is a positive semi-definite Toeplitz weighting matrix with entries that are quadratic in p. Particular choices of D_p result in the maximum likelihood estimator (MLE) if the noise $G - H$ is zero-mean Gaussian with (partially) known covariance, an approximate MLE (AMLE) or the generalized total least squares (GTLS) estimator.

Sufficient conditions for consistency and asymptotic normality for non-Gaussian noise are given in terms of absolute summability of joint cumulants and constraints on the weighting matrix D_p. Expressions for the asymptotic parameter covariance are given and show that the MLE doesn't reach the Cramér-Rao bound.

The Total Least Squares Problem : current state of research and applications.

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The aim of this lecture is to present an overview of the current state of research of a modeling technique which is known as *total least squares* in numerical linear algebra and signal processing, *errors-in-variables* and *orthogonal regression* in the statistical community, *eigenvector or Koopmans-Levin method* and *compensated least squares* in system identification.

The basic motivation for T*otal* L*east* S*quares* (TLS) is the following: Let a set of multidimensional data points (vectors) be given. How can one obtain a linear model that explains these data? The idea is to modify all data points in such a way that some norm of the modification is minimized subject to the constraint that the modified vectors satisfy a linear relation.

The origin of this basic insight can be traced back to the beginning of this century. It was rediscovered many times, often independently, mainly in the statistical and psychometric literature. However, it is only in the last decade that the technique also penetrated in scientific and engineering applications. One of the main reasons for its sudden popularity is the availability of efficient and numerical robust algorithms, in which the *singular value decomposition* plays a prominent role. Another reason is the fact that **TLS** is really an *applications oriented* procedure: It is ideally suited for situations in which all data are corrupted by noise, which is almost always the case in engineering applications. In this sense it is a powerful extension of the classical least squares idea, which corresponds only to a partial modification of the data.

This lecture surveys the TLS problem and enlightens the main results. In particular, the computational, as well as the numerical and statistical aspects of the TLS problem are discussed and compared with those of other related problems, e.g. LS and multivariate regression techniques. Different TLS algorithms are presented and evaluated and practical guidelines are given which delineate the domain of applicability of the TLS method. Furthermore, some recent generalizations of the TLS problem are presented, as well as an overview of its applications.

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An Efficient Total Least Squares Algorithm Based on a Rank-Revealing Two-sided Orthogonal Decomposition.

Sabine Van Huffel[4]

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Solving Total Least Squares (TLS) problems $AX \approx B$ requires the computation of the noise subspace of the data matrix $[A; B]$. The widely used tool for doing this is the Singular Value Decomposition (SVD). However, the SVD has the drawback that it is computationally expensive. Therefore, we consider here a different so-called rank-revealing two-sided orthogonal decomposition which decomposes the matrix into a product of a unitary matrix, a triangular matrix and another unitary matrix in such a way that the effective rank of the matrix is obvious and at the same time the noise subspace is exhibited explicitly. We show how this decomposition leads to an efficient and reliable TLS algorithm that can be parallelized in an efficient way.

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Robust Estimation in Measurement Error Models.

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This talk will discuss the properties of robust estimation for measurement error models. A method for converting ordinary regression algorithms to orthogonal regression algorithms will be described. The main discussion will primarily consider bounded influence estimation using generalized M-estimators. Topics will include sharp lower bounds on the sensitivities, most bounded robust estimators and Hampel's optimality problem. The latter finds estimators which minimize the asymptotic variance subject to an upper bound on the influence function.

Total Chebyshev Approximation.

G. Alistair Watson

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A generalization of the total least squares problem to infinite dimensional spaces is considered, which leads naturally to the total Chebyshev approximation problem:

$$\text{minimize} \| \sum_{i=1}^{n} a_i \phi_i(x) \|_\infty \text{ subject to } \|a\|_2 = 1,$$

where the functions $\phi_i(x)$ are given real functions. Various aspects of this problem are considered.

The Total Least Squares Problem with More than One Solution: Solutions, Perturbation Theory and Relations with the Least Squares Problem.

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This talk presents an analysis of the solutions of the Total Least Squares (TLS) problem $AX \approx B$ in cases where the matrix $[A; B]$ may have multiple smallest singular values. General formulas for the minimum norm TLS solutions are given; the difference between the TLS and the LS solutions is obtained; the error bounds for the perturbed TLS solutions with or without minimal length are deduced. The analysis is useful especially for rank-deficient problems and generalizes the results of Golub and Van Loan, Van Huffel and Vandewalle and Zoltowski. Numerical results for a practical application are also given to verify the error bounds.

WORKSHOP ON

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